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In- and Outbound Spreading of a Free-Particle *s*-Wave

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We show that a free quantum particle in two dimensions with zero angular momentum (s wave) in the form of a ring-shaped wave packet feels an attraction towards the center of the ring, leading first to a contraction followed by an expansion. An experiment to demonstrate this effect is also outlined.

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The spreading of a wave packet is an important topic in quantum mechanics [1]. It arises due to different momenta contained in the packet. As pointed out by Born [2], even a classical ensemble of particles spreads. The only quantum effect lies in the connection between the position and the momentum distributions; that is, the spreads in position and momentum are not independent. In the present Letter we predict a wave effect of the free particle that manifests itself in the dynamics: A ring-shaped wave packet in two dimensions of zero angular momentum feels an attraction towards the center of the ring. This effect, which does not seem to have been noticed previously, is unique to two dimensions and manifests itself for several classes of wave functions.

In order to illustrate this remarkable phenomenon, we first consider the free motion of wave packets in an arbitrary number of dimensions D. One could argue that the investigation in $D > 3$ dimensions has little physical interest, but if we assume that $D = 3N$, where N is the number of particles, the D-dimensional wave packet describes an N-particle system in the ordinary three-dimensional space. We then concentrate on a single particle in two and three dimensions, where we propagate a circular shell and a spherical shell, respectively. All wave packets have initially zero angular momentum and zero average radial momentum. We show that the circular shell first shrinks towards the center and then spreads outwards. In contrast, the spherical shell spreads only outwards. We demonstrate this wave effect unique to two-dimensional space using (i) analytical expressions for the average radial position and momentum, (ii) the Wigner function approach [3] towards quantum mechanics, and (iii) the numerical propagation of wave packets.

Our analytical approach considers the propagation of the initial wave function

$$\Phi_0^{(D)}(x_1, \ldots, x_D) = \frac{\mathcal{N}}{\sqrt{S^{(D)}}} r^2 \exp\left[-\frac{1}{2}\left(\frac{r}{\delta r}\right)^2\right] \quad (1)$$

in the absence of any potential. Here $\mathcal{N} \equiv [2/\Gamma(D/2 + 2)]^{1/2} \delta r^{-D/2-2}$ denotes the radial normalization constant and $r \equiv (x_1^2 + x_2^2 + \ldots x_D^2)^{1/2}$ is the radial variable in D space dimensions. Moreover, $S^{(D)} \equiv 2\pi^{D/2}/\Gamma(D/2)$ is the total solid angle. The quantity δr defines a characteristic length scale of the packet and is a measure of the radial width [4].

In the derivation of our results, we follow two independent approaches that provide identical results: (i) We consider the time evolution in Wigner phase space and calculate the averages with the help of the Wigner function; (ii) we use the method of the generating function [5] to propagate a modulated Gaussian wave packet of the free particle in D dimensions and evaluate the averages. Here we do not present the detailed calculations but only summarize the results [6].

We start by presenting first the general results for the propagation in D dimensions and then focus on the special case of two and three dimensions. It is convenient to introduce the dimensionless time variable

$$\tau \equiv \frac{\hbar t}{\delta r^2 M}, \quad (2)$$

where M denotes the mass of the particle. We find [6] the expression

$$\langle r^{(D)} \rangle(\tau) = \frac{1 + \tau^2/a^{(D)}}{\sqrt{1 + \tau^2}} r_0^{(D)} \quad (3)$$

for the average radial position. Here we have introduced the abbreviation

$$a^{(D)} \equiv 1 + \frac{4D}{D^2 + 3}, \quad (4)$$

and the initial radial position

$$r_0^{(D)} \equiv \frac{\Gamma(\frac{D+5}{2})}{\Gamma(\frac{D+4}{2})} \delta r, \quad (5)$$

in D dimensions, where Γ denotes the Euler gamma function.

Equation (3) shows that for large times the average radial position increases linearly with time, corresponding

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to an expansion of the wave packet. This holds true for any number of dimensions.

For short times we can expand the square root in Eq. (3), which yields

$$\langle r^{(D)}\rangle(\tau) \simeq \left[1 + \left(\frac{1}{a^{(D)}} - \frac{1}{2}\right)\tau^2\right] r_0^{(D)}. \tag{6}$$

An interesting situation occurs when $a^{(D)} > 2$. In this case, the average radius initially decreases, corresponding to a contraction of the wave packet. From the definition Eq. (4) of $a^{(D)}$, we arrive at the contraction condition

$$(D-1)(D-3) < 0. \tag{7}$$

Hence, a contraction occurs only for $D = 2$ corresponding to $a^{(2)} = 15/7 = 2 + 1/7$.

The phenomenon of the contraction can also be viewed by considering the time evolution of the average radial momentum,

$$\langle p^{(D)}\rangle(\tau) = M\frac{d}{dt}\langle r^{(D)}\rangle = \frac{d}{d\tau}\langle r^{(D)}\rangle\frac{\hbar}{\delta r^2}, \tag{8}$$

determined by the time derivative of the average position $\langle r^{(D)}\rangle$, which yields

$$\langle p^{(D)}\rangle(\tau) = -\frac{\tau}{(1+\tau^2)^{3/2}}(a^{(D)} - 2 - \tau^2)\, p_\infty^{(D)}, \tag{9}$$

where

$$p_\infty^{(D)} \equiv \lim_{\tau\to\infty} p^{(D)}(\tau) = \frac{1}{a^{(D)}}\frac{\Gamma(\frac{D+5}{2})}{\Gamma(\frac{D+4}{2})}\frac{\hbar}{\delta r}. \tag{10}$$

The radial momentum is negative, corresponding to a contraction, provided $\tau < [a^{(D)} - 2]^{1/2}$. Since in two dimensions $a^{(2)} = 15/7$, this condition reads $\tau < \tau_{\min} \equiv 1/\sqrt{7}$. At that moment the momentum vanishes and the contraction turns into an expansion. The average radial position assumes a minimum $r_{\min} \equiv \langle r^{(2)}\rangle(\tau_{\min})$.

In order to highlight the special property of two dimensions, we now compare the dynamics of the wave packet Eq. (1) in two and three dimensions. In Fig. 1 we show the time evolution of the average radial position and the average radial momentum in two (solid curves) and three (dashed curves) dimensions based on Eqs. (3) and (9) with $a^{(2)} = 15/7$ and $a^{(3)} = 2$.

For short times the average radius of a ring-shaped wave packet decreases as a function of time. This initial contraction of the circular wave is followed by a final expansion. We emphasize that this phenomenon is not due to an external classical force but occurs for a free particle moving in two dimensions [7]. Obviously the spreading of the ring-shaped wave packet in the radial direction is asymmetric; initially, the probability flux towards the center is larger than towards the outside.

In the three-dimensional case, where we propagate a spherical shell, the average position and the average momentum do not display the soft contraction effect of two dimensions. Indeed, since $a^{(3)} = 2$, the average momentum is always positive and the average position cannot decrease but must increase.

The contraction effect is maximal at $\tau_{\min} = 1/\sqrt{7}$ and, according to Eq. (3), the average radial position $\langle r^{(2)}\rangle$ assumes the minimal value

$$r_{\min} \equiv \sqrt{\frac{224}{225}} r_0^{(2)} \simeq 0.9978\, r_0^{(2)}. \tag{11}$$

Hence, it is a rather soft contraction.

We note that this result is independent of δr, since the problem is scale invariant. But when we choose a different form for the packet, we can make the effect larger. For example, by replacing the prefactor r^2 in Eq. (1) by $\sin(r^2/\delta r^2)$, we obtain at $\tau_{\min} \simeq 1.11$

$$r_{\min} \simeq 0.9964\, \tilde{r}_0, \tag{12}$$

where $\tilde{r}_0$ is the initial average radial position for the new wave function.

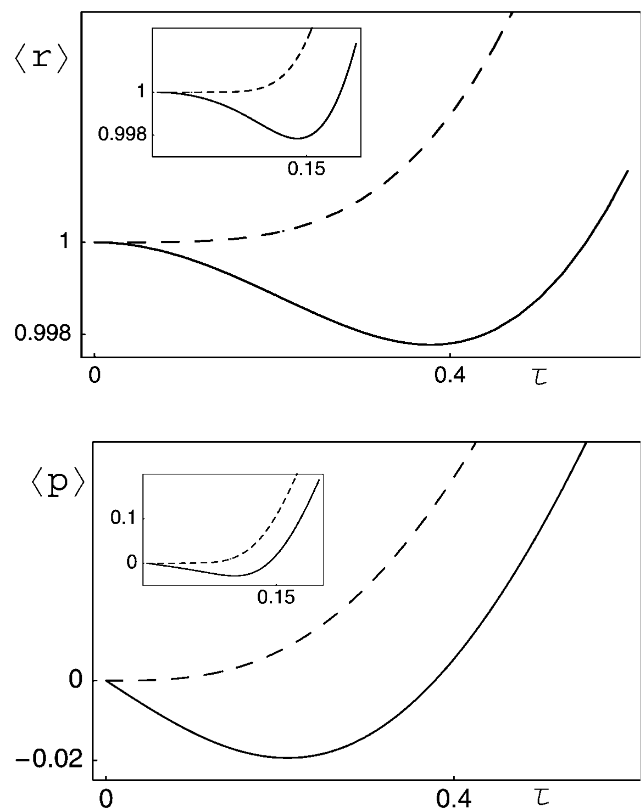

FIG. 1. Comparison between the time evolutions of a circular (solid line) and a spherical shell (dashed line) using the average radial position (top) and the average radial momentum (bottom) obtained from Eqs. (3) and (9) for $a^{(2)} = 15/7$ and $a^{(3)} = 2$. On average the two-dimensional shell first contracts and then expands, whereas the three-dimensional one expands from the onset. In the left insets we show the short time behavior of a displaced Gaussian radial wave packet obtained numerically. Here we have used the same Gaussian for an initial radial wave function in two and three dimensions with $\delta r = 0.4$ and $\rho = 1.5$ in arbitrary units. Position is scaled in units of the initial position $r_0^{(N)}$ of the wave packet and momentum in terms of the final momentum $p_\infty^{(N)}$.

A still larger effect may be obtained by considering a linear combination of two simple Gaussians. We have found that the most favorable function of this type is

$$\Phi(x_1, x_2) = \frac{2.402}{\delta r}\left\{\exp\left[-\frac{1}{2}\left(\frac{r}{\delta r}\right)^2\right] - 0.95\exp\left[-\frac{1}{2}\left(\frac{1.17r}{\delta r}\right)^2\right]\right\}. \tag{13}$$

It leads to the minimal value

$$r_{\min} \simeq 0.9953\tilde{r}_0, \tag{14}$$

obtained at $\tau \simeq 0.394$. The meaning of $\tilde{r}_0$ is similar to the one above. We note that the wave function $\Phi(x_1, x_2)$ has a nonzero value at the origin.

We now turn to the explanation of the contraction effect using the Wigner function [3]. The free particle is one of the few quantum mechanical systems in which the classical phase space dynamics is identical to the quantum mechanical one. Indeed, the Wigner function satisfies the classical Liouville equation. Hence, we find the Wigner function at time t from the Wigner function at time $t = 0$ by replacing the position $\vec{r}$ by $\vec{r} - \vec{p}t/M$. We emphasize that now $\vec{r}$ and $\vec{p}$ denote D-dimensional vectors. The corresponding probability distributions in position and momentum follow by integration over the conjugate variable.

Since for the free particle classical and quantum phase space dynamics are identical, the quantum effect of contraction rather than expansion is stored in the initial Wigner function. To be more precise, it is in the correlations between position and momentum. A classical phase space distribution enjoys a probability interpretation and therefore always has to be positive. In contrast, the Wigner function can assume negative values. Indeed, both the Wigner functions of the circular shell and of the spherical shell contain domains in phase space where they become negative. Since the Wigner function is normalized, the total volume of the Wigner function is unity. We can calculate numerically the volumes $V_-^{(2)}$ and $V_-^{(3)}$ corresponding to the negative parts. We find in the two-dimensional case $V_-^{(2)} \simeq 0.27$, whereas in three dimensions, $V_-^{(3)} \simeq 0.23$. Hence, there is a slightly larger contribution of negative parts in two dimensions than in three dimensions.

In the phase space description of quantum mechanics, quantum effects are stored in the negative parts of the initial Wigner function. Since a classical ensemble of particles cannot have a negative phase space distribution, it cannot display the contraction effect. Needless to say, a classical ensemble with a ring-shaped initial position distribution can show a contraction provided there exists a nonvanishing negative initial radial momentum. However, in our quantum mechanical wave packet, the average radial momentum vanishes.

For the choice Eq. (1) of the initial wave packet, the radial probability density

$$\begin{aligned} W^{(D)}(r)dr &= |\Phi_0^{(D)}(r)|^2 r^{D-1} dr S^{(D)} \\ &= |\mathcal{N}|^2 r^{D+3} e^{-(r/\delta r)^2} dr \end{aligned} \tag{15}$$

depends on the number of dimensions. Hence, one might argue that the contraction is a result of the slightly different initial radial wave functions. In order to exclude this argument, we have performed a numerical integration of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}u_0^{(D)}(r, t) = \left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial r^2} + V^{(D)}(r)\right]u_0^{(D)}(r, t) \tag{16}$$

for the radial wave function $u_0^{(D)}$ of the free particle in two and three space dimensions, corresponding to zero angular momentum. Here we always start with the same initial radial wave function. In this way we guarantee identical radial probability densities in two and three dimensions.

The radial potential

$$V^{(D)}(r) \equiv \frac{\hbar^2}{2M}\frac{(D-1)(D-3)}{4r^2} \tag{17}$$

in D dimensions involves the product $(D-1)(D-3)$ familiar from the contraction condition Eq. (7).

In three dimensions the potential $V^{(3)}$ vanishes. However, for $D = 2$ the quantum anticentrifugal potential

$$V_Q(r) \equiv V^{(2)}(r) \equiv -\frac{\hbar^2}{2M}\frac{1}{4r^2} \tag{18}$$

does not vanish and is negative, that is, attractive [8,9]. This potential is responsible for the contraction.

As already exemplified, a large class of wave packets with zero angular momentum displays this effect of first contracting and then expanding. Indeed, in the inset in Fig. 1 we show the short time evolution of the average radial position and the average radial momentum in two and three dimensions for an initial radial Gaussian wave packet $u(r, t = 0) \equiv \tilde{\mathcal{N}}\exp[-(r-\rho)^2/\delta r^2]$ displaced by an amount ρ from the origin [10]. As in the analytical results, we find a contraction of a circular but not of a spherical shell.

So far we have concentrated on a single particle, but the effect of contraction manifests itself also in the relative motion of two free particles. We can envision the total wave function of the two particles to be of the form Eq. (1) corresponding to an entangled state. When we assume that each particle is allowed to move in a d-dimensional space, the total wave function lives in a $D = 2 \cdot d$-dimensional configuration space. The physical situation of a single particle contracting in two dimensions corresponds to two particles constrained to one dimension. When they move along a line, their average relative separation first decreases and then increases. It looks like the particles first attract and then repel each other. However, when they move in two or three dimensions, their relative distance always increases.

We conclude by briefly outlining an experiment to demonstrate the contraction effect. At first sight, one might think of cold atoms around a wire familiar from atom chips [11]. However, it might be easier to make use of the analogy between the Schrödinger equation and the paraxial wave equation of classical electrodynamics. We shine monochromatic light onto an opaque screen with an annular aperture. In order to avoid diffraction from sharp edges, we introduce apodization, that is, a position dependence transmission coefficient. At the edges of the ring almost no light is transmitted, whereas at the center of the ring almost all light passes through. This arrangement creates an intensity distribution after the screen confined mainly to a ring. The subsequent free propagation in space is analogous to the free propagation in time of the Schrödinger wave function. The time dependent probability distribution then corresponds to the transverse intensity distributions at different locations downstream from the screen [12].

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